D-Aspartic acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C17H31NO6/c1-8-22-17(21)18-14(16(20)24-13(7)11(4)5)9-15(19)23-12(6)10(2

InchiKey: KWVPQXWGXJGACE-ROKHWSDSSA-N

Formula: C17H31NO6

SMILES: CCOC(=O)NC(CC(=O)OC(C)C(C)C)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 345.43

Physical Properties

Property code	Value	Unit	Source
gf	-532.31	kJ/mol	Joback Method
hf	-1101.54	kJ/mol	Joback Method
hfus	35.63	kJ/mol	Joback Method
hvap	85.40	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.667		Crippen Method
mcvol	282.690	ml/mol	McGowan Method
pc	1414.37	kPa	Joback Method
rinpol	2010.50		NIST Webbook
tb	865.20	K	Joback Method
tc	1065.66	K	Joback Method
tf	475.49	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.19	J/mol×K	865.20	Joback Method
cpg	920.29	J/mol×K	898.61	Joback Method
cpg	934.14	J/mol×K	932.02	Joback Method
cpg	946.76	J/mol×K	965.43	Joback Method
cpg	958.14	J/mol×K	998.84	Joback Method
cpg	968.28	J/mol×K	1032.25	Joback Method
cpg	977.19	J/mol×K	1065.66	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R501801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume